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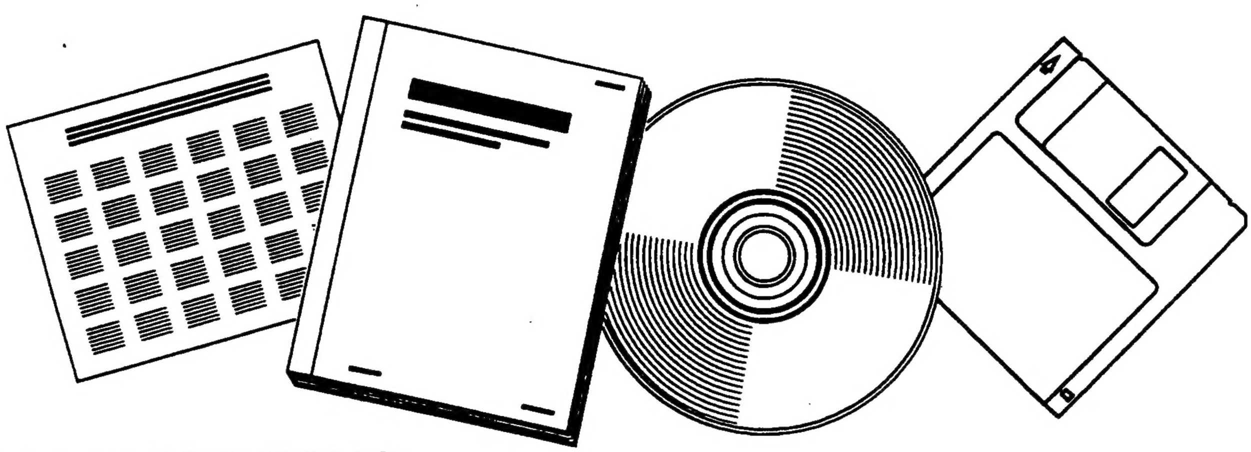
A REVIEW OF GROUND WATER MODELING NEEDS FOR THE U.S. ARMY

WATER SCIENCE AND TECHNOLOGY BOARD
WASHINGTON, DC

SEP 92



U.S. DEPARTMENT OF COMMERCE
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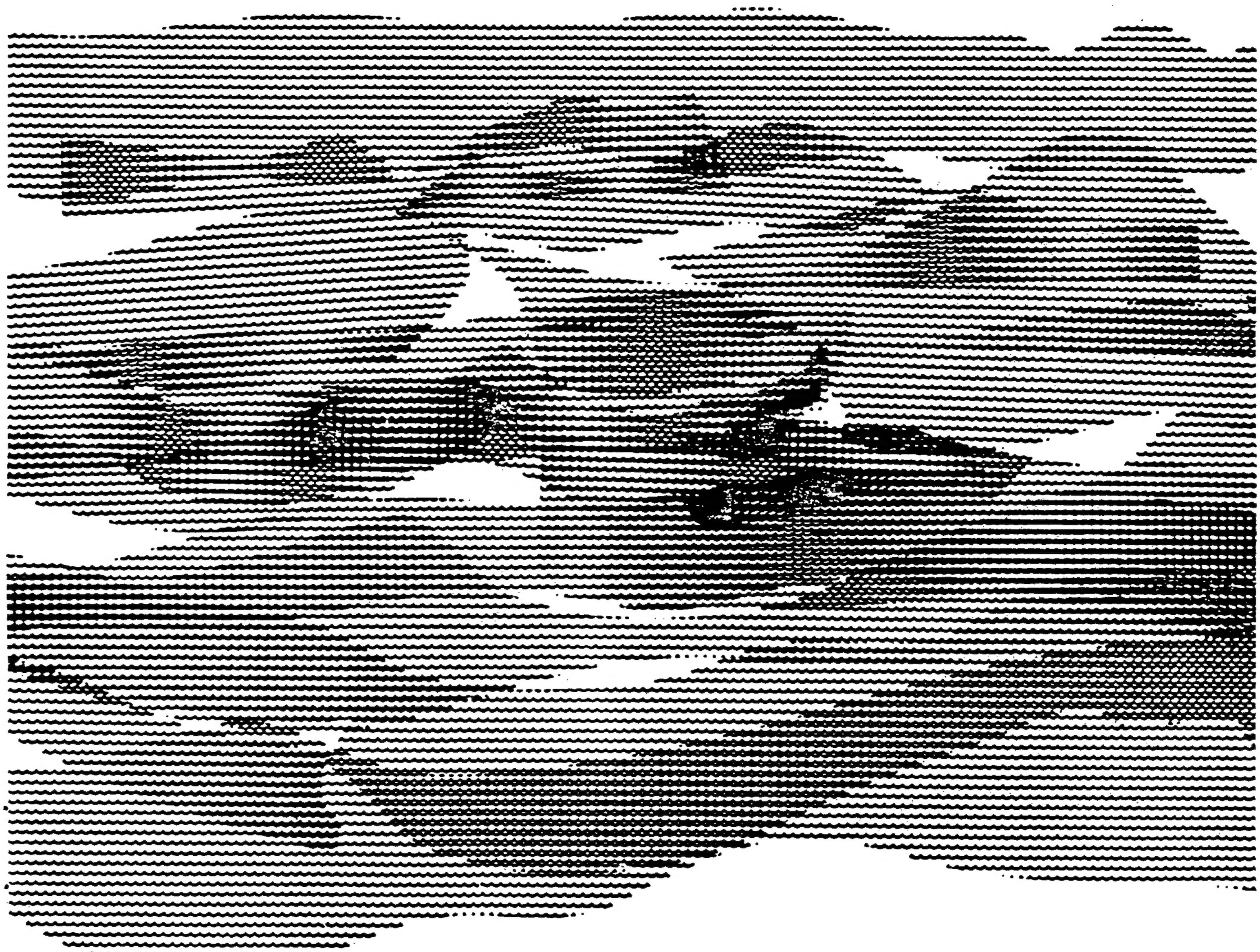

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A Review of Ground Water Modeling Needs for the U.S. Army

Water Science and Technology Board
Commission on Geosciences, Environment, and Resources

September 1992
National Research Council
Washington, D.C.

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Support for the project was provided by the U.S. Army Corps of Engineers under Agreement Number DACA 39-92-K-0019/C.

Available from
Water Science and Technology Board
National Research Council
2101 Constitution Avenue, N.W.
Washington, D.C. 20418

Printed in the United States of America

50272-101

REPORT DOCUMENTATION PAGE	1. REPORT NO.	2.	3. PB93-146322

4. Title and Subtitle A Review of Ground Water Modeling Needs for the U.S. Army	5. Report Date
	6.
7. Author(s) Water Science and Technology Board Commission on Geosciences, Environment, and Resources	8. Performing Organization Rept. No.
9. Performing Organization Name and Address Water Science and Technology Board National Research Council 2101 Constitution Avenue, NW Washington, DC 20418	10. Project/Task/Work Unit No.
	11. Contract(C) or Grant(G) No. (C) DACA39-92-K-0019/C (G)
12. Sponsoring Organization Name and Address U.S. Army Corp of Engineers	13. Type of Report & Period Covered
	14.

15. Supplementary Notes

16. Abstract (Limit: 200 words)

A Review of Ground Water Modeling Needs for the U.S. Army addresses the magnitude of ground water contamination at Army installations. The study recommends that the Army develop in-house expertise in ground water modeling, expand partnership programs between the Army and academic researchers, and develop a ground water modeling support center to help focus research, technology transfer and training activities.

17. Document Analysis a. Descriptors

b. Identifiers/Open-Ended Terms

c. COSATI Field/Group

18. Availability Statement Release unlimited	19. Security Class (This Report)	21. No. of Pages 39
	20. Security Class (This Page)	22. Price

(See ANSI-Z39.18) *See Instructions on Reverse* OPTIONAL FORM 272 (4-77) (Formerly NTIS-35) Department of Commerce

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Preface

The U.S. Army has identified over 10,000 potentially contaminated sites at Army installations. Many of these sites will involve contaminated ground water. A fundamental understanding of ground water flow and contaminant transport processes, and the ability to predict these processes, are prerequisites to designing remedial actions for contaminated sites. There is a need for a ground water science and technology program to support the Army's remediation efforts, including a strong capability for mathematical modeling. The Army Corps of Engineers Waterways Experiment Station (WES) is the lead research and development laboratory for supporting the Army's ground water remediation activities. With this in mind, WES asked the Water Science and Technology Board (WSTB) to conduct an evaluation of the state of the art in ground water flow and contaminant transport modeling and to provide advice on how the Army's needs in this area might be met.

To provide this advice, the WSTB hosted a workshop on June 30-July 1, 1992. During the workshop, Dr. Jeffrey P. Holland (WES) presented an overview of WES and the Army's needs in ground water modeling. Participants reviewed the nature of contaminant problems at Army sites and discussed the results of a recent Army workshop on ground water modeling. The group relied on the presentation at the workshop for most of the information about the Army's modeling activities and did not investigate them in detail.

Given WES's need for a prompt evaluation, the WSTB assembled a study group of experts on ground water modeling to participate in the workshop and contribute to this report. All the participants were involved with the board's study *Ground Water Models: Scientific and Regulatory Applications*, published in 1990. The group included several board members (all of whom were on the study committee): David L. Freyberg, who chaired the workshop, Stanford University; Bruce E. Rittmann, University of Illinois; and Donald D. Runnells, University of Colorado. The group also included other individuals who were involved in the 1990 effort (as members of either the committee or the board at the time) -- Mary P. Anderson, University of Wisconsin-Madison; James W.

Mercer, GeoTrans, Inc.; and Frank W. Schwartz, The Ohio State University. Stavros Papadopulos, S.S. Papadopulos and Associates, Inc. helped to organize this review and refine the report. The project was managed by Gary D. Krauss, staff officer of WSTB, with help from Greicy Amjadivala, project assistant. Robert Katt provided editorial assistance. The board is very grateful to these individuals, but takes full responsibility for the content of this report.

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Executive Summary

This report was prepared to assist the U.S. Army in remediation of ground water contamination from hazardous, toxic, and radioactive wastes at Army installations. The Waterways Experiment Station of the Army Corps of Engineers requested that the Water Science and Technology Board evaluate the state of the art in mathematical models of ground water flow and contaminant transport, and then advise the Corps of Engineers on how it might support and use such models to meet Army's ground water remediation needs over the next ten years.

To characterize the technical capabilities in modeling, the report distinguishes three stages of progress toward the ultimate goal of producing a useful, site-specific model of the processes that control ground water flow and contaminant transport. During *discovery*, a physical process is characterized to the point of allowing an initial mathematical formulation. In the subsequent *description* stage, studies are performed to detail how the process works, to relate it to other processes, and to determine values for its controlling parameters. These studies may entail laboratory and carefully controlled field experiments, as well as mathematical manipulations such as sensitivity analyses. Only after the process and its controlling parameters are understood well enough to assure that the mathematical description accurately represents their real behavior can the model advance to the third stage of *application*.

This three-stage framework is used in Chapter 2 to characterize the state of knowledge for the following physical and chemical processes:

- *flow processes*–saturated, unsaturated, or multiphase flow through porous media;
- *mass transport and chemical mass transfer processes*– advection/dispersion, radioactive decay, biological processes, and multiphase interactions such as sorption, oxidation-reduction, and precipitation dissolution; and
- *other processes*–including coupled flow processes and flow/transport in fractured media.

For some of these processes, including saturated flow in porous media, advection/dispersion, and radioactive decay, the state of knowledge is at or near the application stage. More complex processes, such as multiphase flow in porous media or coupled flow, are barely beyond the discovery stage. The analysis of existing capabilities ends with a table of references for recent advances in modeling, which updates the board's 1990 study on ground water models.

Based on a review of the state of knowledge and a preliminary understanding of Army needs, the board recommends that the Corps of Engineers take the following actions:

- Develop sufficient expertise in ground water modeling to support a successful in-house capability.
- Undertake field-scale research and testing of model applications.
- Investigate the physical, chemical, and biological processes occurring in subsurface contamination with explosives, since these contaminants are less likely to be studied by other agencies and may have unique problems.
- Investigate the contamination of cold climate sites, since this situation is also less likely to be studied elsewhere.
- Apply the Army's state-of-the-art experience in user-friendly interfaces to develop excellent user-model interfaces for ground water models.
- Expand the programs and activities through which the Army and the Corps of Engineers build long-lasting partnerships with academic researchers who do the fundamental research on the physical, chemical, and biological processes of ground water remediation.
- Develop a ground water modeling support center for research, technology transfer, and training.

In the board's judgment a research program in the application of ground water modeling to the Army's remediation efforts would be best supported by developing a center for research and training. Given the actions to be taken and the interests and support facilities already present at the Waterways Experiment Station, it is in an excellent position to serve in this role.

1

Introduction

In the past decade, the contamination of ground water has been recognized as a significant environmental and public health threat in the United States and throughout the world. Included among those organizations confronting this problem is the U.S. Army. The Army has identified 10,578 individual sites, located in 1,265 active installations that are potentially contaminated by hazardous, toxic, and radioactive materials (Defense Environmental Restoration Program, Annual Report to Congress for Fiscal Year 1991, February, 1992). Through initial investigations, the Army has determined that 5,054 sites require no action. Of the remaining 5,524 sites that require further study and possible cleanup, the Army has studied only a small percentage. It is anticipated that many of these sites will have ground water contamination. This large number of sites, combined with the ambitious goal of cleaning them up by 2012, places great pressure on Army personnel responsible for cleanup to understand ground water problems and to be able to design appropriate solutions. Part of this understanding involves the use of ground water models.

The U.S. Army Toxic and Hazardous Materials Agency (USATHAMA) is the responsible agency for managing what is known within U.S. Department of Defense (DOD) as "installation restoration," which includes ground water remediation activities. For several years the U.S. Army Corps of Engineers (USACE) Waterways Experiment Station (WES) has been the lead research and development laboratory for Army installation restoration. Along with WES, two other Army research labs -- the Cold Regions Research and Engineering Laboratory (CRREL) in Hanover, New Hampshire, and the Construction Engineering Research Laboratory (CERL) in Champaign, Illinois -- support USATHAMA in its restoration efforts. Most of the efforts to date have been focused on detecting and monitoring contamination. It has become clear, however, that ground water models are among the most important scientific tools available for understanding ground water processes. Numerical simulation models have been used extensively to estimate the rates of ground water flow and contaminant migration, identify potential receptors of contaminated ground water, and design remedial systems at numerous hazardous waste sites. Additional research and model development is still

needed, especially for models that deal with complex heterogeneities, fractured media, multiphase flow, and the transport and fate of chemicals in the subsurface. As a result, WES is increasing its role in the modeling of ground water flow and contaminant transport.

Although WES has a considerable history in hydraulics, geotechnology, structures, surface water quality, ecology, and coastal engineering, its experience in ground water modeling is limited. In an effort to obtain guidance concerning the Army's ground water modeling effort, WES asked the Water Science and Technology Board (WSTB) for assistance. Specifically, WES asked WSTB to update its report *Ground Water Models: Scientific and Regulatory Applications* (NRC, 1990), a comprehensive assessment of the state of the science at that time, and to identify modeling issues that the Army should deal with over the next 10 years.

The goal of this report is to assist the U.S. Army in responding to ground water contamination problems associated with waste activities at Army installations. In particular, the report provides guidance to the Army as it considers the development of its capabilities for research, testing and evaluation, and especially the application of ground water flow and transport simulation models at sites with spills, residual contamination, and ground water remediation actions. The report includes three chapters. This chapter introduces the goals of the report. Chapter 2 describes the role of ground water modeling and gaps in the state of knowledge of modeling ground water processes. Chapter 3 presents recommendations to the Army for filling some of the gaps in the state of knowledge with particular relevance to Army needs.

The recommendations reflect the study group's knowledge with respect to current, world-wide research activities, its general understanding of the Army's role and capabilities in the area of ground water remediation and modeling, and an awareness of the Army's unique position of control over restricted sites for testing and experimentation. The recommendations are aimed at making efficient use of the Army's scientific and technological resources to advance the state of knowledge with the participation of the civilian scientific community. The report proposes the formation of an Army in-house support center to focus research and technology transfer activities and to coordinate external partnerships and contracting activities. The report also identifies expertise needed for ground water modeling in the Army, provides guidance on modeling development, and gives suggestions for specific areas of ground water research and technology transfer activities. The report identifies the essential ingredients -- research, expertise, and support -- for the Army's successful development and application of a ground water modeling capability.

2

Ground Water Models: Gaps in the State of Knowledge

ROLE OF GROUND WATER MODELING

Mathematical models play many roles in ground water science and technology. They serve the important function of codifying knowledge of the physical, chemical, and biological processes that control the transport and fate of contaminants in ground water. In practical, site-specific applications, mathematical models function as important decision-making tools. In this role, models are used to reduce the uncertainty inherent in decision-making by providing a rational, logical, self-consistent structure for data collection, site characterization, hypothesis testing, quantification of uncertainty, risk assessment, and the design and evaluation of corrective intervention or remedial actions.

During site characterization, a hypothesis or conceptual model is formulated through a preliminary understanding of physical, chemical, and biological processes. Based on this conceptualization, a data collection program is designed and implemented. As new data and information become available, the site conceptualization is updated and the need for additional data is determined. Thus, site characterization is an iterative process. The conceptualization often is incorporated into a numerical ground water model to keep track of all the necessary site information effectively, and to insure that the conceptualization is self-consistent and reflects current knowledge of physical, chemical, and biological processes. In this manner, use of the model can help guide both system conceptualization and data collection activities.

The model subsequently can be used to help identify pathways and potential receptors, which is the exposure assessment portion of a risk assessment. Solute transport models, for example, can be used to compute concentration versus time at the receptors. Ground water models can also be used to evaluate the effectiveness and associated risk reduction of proposed ground water remediations before they are implemented. This can include the effects of wells, drains, and permeability barriers. In this way, models can aid in the selection and design of remediation techniques. Once the remediation is implemented, models can be used to help evaluate and improve operation

of the remedy. Finally, models can be used to help estimate the impact of terminating the remediation. This could, for example, take the form of an Alternative Concentration Limit (ACL) evaluation, where models are used to show the impacts of reducing contaminants to a specified concentration by cleanup.

THE EVOLUTIONARY STAGES IN MODELING GROUND WATER PROCESSES

Mathematical modeling of ground water systems is an attempt to take an understanding of real world processes and represent it in mathematical terms (NRC, 1990). Over time, hydrogeologists have recognized that the evolution of process models follows a well-defined pathway that leads from process discovery to process description and finally to process application. The first step in developing a mathematical model of a process is the initial discovery of the process and its mathematical formulation. The actual discovery can come from observations made from experiments or field studies, but discoveries can also come about through theoretical analyses.

After a process has been discovered, significant time and energy are expended in process description. During this stage in the evolution of a process model, studies are designed to show in detail how the process works, to determine the importance of one process relative to other processes, and to establish values for characteristic parameters of the process. Typically, process description is accomplished mainly through carefully controlled field and laboratory experiments, and sensitivity analyses with mathematical models.

When a process and its controlling parameters are well understood, it is possible to use process models to solve practical problems. In effect, the implicit assumption is made that the mathematical description of the process accurately represents the behavior of a real system. The model is put into practice through computer software, often enlisting the aid of numerical analysts to develop the software code from the relevant mathematical equations.

When models are applied as predictive decision-making tools to reduce uncertainty, the limitations or gaps in the state of knowledge usually involve the appropriate application of a model to site-specific conditions, including identifying whether or not the development of a new or refined model is required. The relationship between predictive uncertainty and the amount, location, and type of data available at a site is poorly understood. The establishment of appropriate parameter values for a model, based on available data and the required level of predictive uncertainty, is also a challenging, incompletely understood task. Scaling relationships between process knowledge acquired in the laboratory and its representation and parameterization in models applied over field dimensions must be understood for physical, chemical, and biological processes. Efficiently assessing which processes are important and relevant to successful decision-making at a particular site is a critical, yet elusive, art.

One important benefit of model-based studies of processes is that key parameters controlling the process are clearly identified for further work. In most cases, the work that is identified revolves around developing theoretical, experimental, and field-based

approaches for estimating the values for model parameters. Because both the complexity of processes and our knowledge of them vary, it should come as no surprise that there is also broad variability in our state of knowledge with respect to model parameters.

In practice, it is the spatial and temporal variability in the model parameters that represent the essence of the particular flow and transport conditions at the site. Lack of knowledge concerning this parameter variability is a major source of prediction error, or uncertainty, in model predictions. This lack of knowledge is due, in large part, to insufficient site characterization, and has become a major impediment in the successful use of models. It is for this reason that the pursuit of knowledge to improve our understanding of parameters, and the methods used to define the parameters in the field, represents legitimate and important research initiatives. Clearly, some parameters are more difficult to evaluate than others. Because of limits to site data, modeling research should also consider the determination of methods to allow decisions where data are limited.

Effectively managing data and the development of a people/model interface for information retrieval and model input/output are also enormous challenges related to process application. These issues of process application will dominate many of the practical problems facing the Army and provide many of the opportunities for the Army to contribute to the advancement of science as it develops its ground water management capabilities.

One can use the idea of evolutionary stages as a measure of the state of knowledge of particular processes. Some hydrogeological processes, such as ground water flow in relatively homogeneous porous media, have been studied for more than 100 years and have been in an application stage for many years. Other processes are much less well known and in many respects are just now being described. An assessment of progress with respect to some of the most important processes contributing to contaminant transport and fate is summarized in Table 1. The list of processes is divided into three parts, representing (1) a set of flow processes, (2) a set of mass transport and chemical mass transfer processes, and (3) a set of other, generally more complicated processes. This latter category represents complexities in the manifestation of processes due to fractures and coupling among the flow and transport processes.

In Table 1, the status of modeling is graphically depicted by a series of dots centered under the appropriate State of Knowledge -- Discovery, Description, or Application -- where the bulk of activity resides. The center of activity is represented by two heavy dots, with the lighter dots representing the ranges of activities.

Saturated Flow - Porous Media

The first group of processes includes both single and multiphase flow through porous media. As Table 1 illustrates, the state of knowledge with respect to the saturated flow of ground water in porous media is well developed with the bulk of the activities at the applications end. This finding should come as no surprise because understanding flow through porous media formed the scientific basis of hydrogeology

TABLE 1 Progress in Modeling

Process	State of knowledge		
	Discovery	Description	Application
Flow processes			
saturated flow - porous media			. . . ● ● .
unsaturated flow - porous media		. . .	● ● . .
multiphase flow - porous media	.	. ● ●	.
Mass transport and chemical mass transfer processes			
advection/dispersion		.	. ● ● . . .
radioactive decay			. . ● ●
biological processes	.	. ● ●	. . .
multiphase interactions	.	. ● ● . . .	
Other processes			
coupled flow processes	●	● . . .	
flow/transport - fractured	●	●	.

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from the pioneering efforts of Darcy, Slichter, and Chamberlin in the 1800's, to Meinzer and Theis (1935) in the early part of this century, through the defining studies of well hydraulics and its applications by Jacob and Hantush in the 1940's, 50's and 60's, and ultimately to work on regional ground water flow by Hubbert (1940), Toth (1962; 1963), and Freeze and Witherspoon (1966; 1967). The late 1960's saw the beginning of the computer revolution where the pioneering work of Pinder and Bredehoeft (1968), and Pinder and Frind (1972) formed the basis for the powerful modeling tools we now routinely use in hydrogeological practice.

Continuing work in this area is practical in nature and mainly designed to improve the efficiency and robustness of existing codes, to offer useful embellishments, and to improve the usability of the codes through pre- and post-processors. Modest efforts by industry and government should enable the models to keep in step with increasing hardware and software capabilities. However, site characterization and parameter uncertainty remain as important challenges for site-specific application.

Unsaturated Flow - Porous Media

This specific flow problem involves the flow of a single fluid -- water -- and assumes that the gas phase is connected to the atmosphere and is not modeled explicitly. The resistance that the gas phase offers to flowing water is incorporated in the modeling process through the hydraulic conductivity term. Traditionally, work on this problem has resided in the domain of soil physicists concerned with local scale fluxes of water in the vadose zone (the region between the soil surface and the water table). Paralleling the experience in saturated systems, there is a long and rich history of fundamental and applied modeling of unsaturated flow in porous media.

Mathematically, the approach to modeling the flow of water in an unsaturated medium is more complicated than the analogous case for saturated flow. Hydraulic conductivity, which is constant for saturated flow, varies as a function of moisture content and therefore pressure head. Thus, there is a requirement for additional information in the form of soil hydraulic conductivity curves (hydraulic conductivity versus pressure head), and soil-water characteristic curves (soil moisture versus pressure head) (NRC, 1990). Because the resulting equation of flow is in general nonlinear, the possibilities of analytical modeling of flow are limited to steady flow and, for unsteady flow, to exponential hydraulic conductivity curves that lead to linearized forms of the flow equation (e.g., Srivastava and Yeh, 1991). Numerical solutions to some forms of the unsaturated flow problem have existed for many years (e.g., Freeze, 1969; Freeze, 1971).

Experience with parameters and the solutions to the nonlinear flow equation have made the application of unsaturated flow models relatively routine for problems involving homogeneous porous media (assuming data are available). The main focus of research is now on problems involving heterogeneity, such as dual porosity systems that develop due to the presence of fractures or macropores. Questions remain about the theoretical treatment of the coupling between the matrix and fracture systems, and the form of characteristic curves for large macropores. One of the most extensive research programs

in this respect is work that is under way with the Yucca Mountain Project in Nevada (Dudley et al., 1985; Dykhuizen, 1990; Nitao and Buschek, 1991; Prindle and Hopkins, 1989).

Opportunities for research remain in this field, including improvements in numerical methods and proper parameterization for field-scale applications. Unsaturated flow problems remain computationally burdensome and field-scale characterization is not yet well understood.

Multiphase Flow - Porous Media

The term multiphase flow in hydrogeology applies generally to the simultaneous flow of water and other liquids or gases. Examples of these problems include the flow of a nonaqueous phase liquid (NAPL) such as gasoline in a medium that is saturated or partially saturated with water, or simply the flow of water and gases in the unsaturated zone.

A significant capability for multiphase modeling was developed originally in the petroleum industry to assist engineers in the exploitation of oil and gas reserves. However, it was not until the early 1980's that hydrogeologists became aware of the significance of contamination due to NAPL's and the need for process models. The years of detailed work in the petroleum industry provided an important theoretical and methodological framework that promoted the rapid early evolution of modeling capabilities. However, it soon became clear that the NAPL problem in ground water offers unique challenges in theory and modeling methods because of the range in properties that organic liquids can possess and the need to consider complex interphase mass transfers due to volatilization or dissolution of some compounds.

The main approaches to modeling NAPL flow (as described in NRC, 1990) are sharp interface approaches (Hochmuth and Sunada, 1985; Schiegg, 1986; and van Dam, 1967); immiscible phase approaches incorporating capillarity (e.g., Faust, 1985; Osborne and Sykes, 1986); and compositional models that incorporate interphase transfer (e.g., Abriola and Pinder, 1985a,b; Baehr and Corapcioglu, 1987). In terms of applications, immiscible phase approaches are used most extensively, while the compositional model approach shows the greatest potential for problems involving multiple chemicals that need to be tracked. The lack of experience in characterizing multiphase flow parameters relevant to contaminant systems has meant that process models are not now widely used in practice. There is nonetheless a history of modeling experience in industry with the immiscible approaches, using computer models such as SWANFLOW (Faust, 1985; Faust et al., 1989b) and ARMOS (Parker et al., 1990). However, as shown in Table 1, there is need for considerably more work before the modeling technology evolves to the application stage. The main limitation of these models is the lack of site-specific data.

Although it is beyond the scope of this report to review in detail the potential directions of research needed to model multicomponent flow, there remains a continuing need for experience in describing the flow characteristics of various media at the laboratory and field scales, particularly as influenced by the unique compositional and

chemical characteristics of organic contaminants. In addition, codes need to be made more usable commercially through appropriate user interfaces and documentation of sample problems.

Advection and Dispersion

Advection and dispersion together account for the physical transport of mass from one point to another in a ground water system (Domenico and Schwartz, 1990). The mathematical basis for representing mass transport processes -- particularly dispersion -- grew from theoretical studies by Scheideger (1954) and de Jong (1958), among others. The integrated mathematical description of advection and dispersion came later in work by Bear (1972) and Bredehoeft and Pinder (1973). Although the mathematical framework for describing these processes has been in place for more than two decades, only in the last few years have the processes themselves been understood with any confidence.

The theoretical difficulties have centered on deciphering the nature of dispersion at various scales. Both theoretical studies (e.g., Gelhar and Axness, 1983, Smith and Schwartz, 1980) and large-scale field experiments (e.g., Mackay et al., 1986, Freyberg, 1986; Sudicky, 1986; Boggs et al., in press) have contributed to this effort.

In practice, a variety of mathematical approaches have been used in modeling advection and dispersion. Analytical approaches often are adequate for simple problems and have formed the basis for practical inverse methods (Domenico and Robbins, 1985; Ala and Domenico, 1992). More complex problems require numerical approaches that are embodied in computer models such as MOC (Konikow and Bredehoeft, 1978) and MT3D (Zheng, 1990).

Theoretical process studies have begun to dwindle, but significant research is continuing in the development of sophisticated numerical approaches to overcome limitations with the current generation of computer models. For example, the development of orthogonal minimization solvers by workers at the University of Waterloo (e.g., Mendoza and Frind, 1990) and the U.S. Geological Survey (Rubin, 1992) have made it possible to work on large three-dimensional problems that were beyond the capabilities of earlier generations of computer models. Work is also under way to develop comprehensive simulation packages built around the MODFLOW model such as MT3D (Zheng, 1990).

Work clearly remains to be done in this area. As is the case with saturated and unsaturated flow, most activity will be in the area of the application of models and refinement of field techniques to measure parameters required by the models. Software will increase the ease of using existing models through pre- and post-processors.

Radioactive Decay, Biological Processes, and Multiphase Interactions

As mass is transported through a ground water system, it can be influenced by nuclear, chemical, and biological processes. The chemical mass transfer processes listed in Table 1 are not exhaustive but are simply examples of the chemical processes pertinent to contaminant problems. A more comprehensive discussion of inorganic chemical processes in ground water is presented by Runnells (in press). As Table 1 suggests, a few simple processes such as radioactive decay are well known and can be modeled with relatively little uncertainty. Several other transport processes, such as biological processes and multiphase interactions, are generally less well known. Work to describe these processes is the focal point of much of the present-day research in contaminant hydrogeology.

Generally speaking, most of the key nuclear, chemical, and biological processes are relatively well understood. There are valid mathematical representations of the processes that involve biotransformation, surface reactions, or mineral dissolution/precipitation reactions. However, fundamental gaps in knowledge still exist in describing the complex interactions that may occur among constituents, for example, co-solvent effects in surface reactions, interactions among several biological substrates, mixtures of inorganic substrates in real aquifers, oxidation-reduction reactions, or solid solution in precipitation/dissolution processes. Thus, representation of the state of knowledge in modeling these processes in Table 1 includes a small component of discovery.

The main impediment to evolving past the descriptive phase is the broad diversity and complexity in biological systems and in chemical reactions involving organic and inorganic chemicals. In the case of biological reactions, the base of descriptive knowledge is sufficient to predict the fate of only a few common contaminants under relatively simple geochemical conditions. Data necessary to model the kinetic character of biological and inorganic reactions are sparse. Although considerable research is needed to fully understand the operation of biological systems, transport models have attempted to include some biological effects. The simplest models represent the biotransformation of organic compounds as a first-order kinetic process (e.g., Bouwer and McCarty, 1984). Other more mechanistic transport models (e.g., Borden and Bedient, 1986; Molz et al., 1986, Odencrantz et al., 1990) incorporate kinetic models of the microbial populations. However, the kinetic (and other necessary) parameters for these formulations are poorly known, and there has been little field scale validation of the approach.

In terms of surface reactions, the problem of parameterizing the system is a little less severe. For one, there exists an extensive base of information on the equilibrium partitioning of hydrophobic organic compounds, which preliminary testing shows to work reasonably well in ground water systems (Curtis et al., 1986). A second reason is the belief that for engineering decisions, metal sorption can be modeled using site-specific estimates of distribution coefficients. However, it is generally conceded that the K_d approach to modeling the surface behavior of metals is weak (Domenico and Schwartz, 1990). Attempts to move to more sophisticated process models (e.g., surface

complexation or cation exchange) or to kinetic representations of processes in real aquifers are again frustrated by a lack of data for geological systems.

Another type of multiphase process involves the redistribution of mass among the solids, other liquids, and gases that water encounters in moving through a ground water system. The simplest models of these processes are based on equilibrium mass law relationships for which a relatively complete data base of equilibrium constants is available. However, if the reactions of interest are best described using a kinetic viewpoint, then virtually no data exist.

The state of practice in the application of transport models that can account for nuclear, chemical, and biological processes has advanced very little in recent years. Typically, most codes work with a small subset of the possible reactions, and they avoid nonlinear kinetics expressions through the use of first-order kinetic rate laws for biotransformation reactions and simple Freundlich models for sorption. The kinetics of oxidation-reduction reactions in ground water are also poorly known (Lindberg and Runnells, 1984). More comprehensive codes have been developed (e.g., Liu and Narasimhan, 1989); however, they have rarely been used in solving practical problems. BIOPLUME (Rafai and Bedient, 1990) is one example of a code that includes advection, dispersion, and biological reactions. Although the biological reaction term is not sophisticated, it seems to be adequate for modeling on large spatial scales, and the code has been used successfully in practice for modeling the cleanup of petroleum hydrocarbons. Beyond the problem of collecting the necessary data to use the more complex models at a site, a more fundamental research need is to validate the relevant governing equations at both the laboratory and field scales.

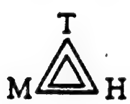
The NRC's 1990 study discussed at length the need for ongoing research to represent geochemical processes more accurately in transport models. While research has continued, significant progress on a variety of fronts will still be required before such models can be used routinely in applications. In particular, advances are needed in determining the kinetics of relevant reactions, controlling factors in oxidation-reduction processes, and modeling of sorption reactions involving realistic aquifer substrates.

Coupled Flow Processes

The term "coupled flow processes" is used here to mean complex problems of flow and transport where, for example, the flow of water depends strongly on the concentration distribution, which in turn depends on the flow of water. In even more complex situations, flow depends on both mass and energy transport. Indeed, as Table 2 illustrates, there are many different examples of coupling among thermal, hydrologic, mechanical, chemical, and biological processes.

Progress in the mathematical modeling of these kinds of problems has been mixed. For certain problems, like the interaction between fresh water and sea water, there have been considerable efforts in model development. However, in general, progress in the modeling of complex coupled processes is relatively limited. The most

TABLE 2 Types of Coupled Processes

No.	Type	Example
1.	T = C	phase changes
2.	T = H	buoyancy flow
3.	T = M	thermally induced fractures
4.	H = C	solution and precipitation
5.	H = M	hydraulic fracturing
6.	C–M	stress corrosion
7.		chemical reactions and transport in hydrothermal systems
8.		thermomechanical effects with change of mechanical strengths due to thermochemical transformation
9.		thermally induced hydromechanical behavior of fractured rocks
10.		hydromechanical effects (in fractures) that may influence chemical transport
11.		chemical reactions and transport in fractures under thermal and hydraulic loading

Note: T = Thermal, M = Mechanical, H = Hydrological, C = Chemical. A single line indicates weak coupling; a double line indicates strong coupling.

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serious modeling effort in the area of coupled flow is in relation to the problems accompanying nuclear waste disposal. A good overview of the theoretical and experimental work on this topic is provided in the 1985 proceedings of a conference on coupled processes (Tsang, 1987). Applied work is continuing, for example, with the code V-TOUGH as part of the Yucca Mountain program to develop mathematical models to predict the response of the hydrologic system to significant repository heating (Nitao et al., 1992).

For more conventional problems of ground water contamination, work is just beginning to examine coupled processes. Examples include the modeling of density-driven transport of hydrocarbon vapors in partially saturated media (Mendoza and Frind, 1990a,b) and the experimental modeling of unstable mixed flows (Schincariol and Schwartz, 1990; Oostrom et al., 1992). Coupled process models have not been needed because, to date, simpler transport models have proven to be adequate for many applications.

Coupled process modeling is emerging as a fertile area for theoretical research. The complexity of coupled systems makes it difficult to anticipate results, so careful systematic studies are required. The field has been slow to develop in part because of the high level of sophistication necessary in the codes for solving systems of partial differential equations and in part because of the tremendous computational power required to solve even relatively small problems. Run times of days on state-of-the-art workstations, and many hours on supercomputers, are the norm for even simple problems. There are efforts under way to develop alternative approaches, such as lattice gas methods that can take advantage of parallel computer architectures, but this work remains in its infancy.

Flow and Transport in Fractured Media

Problems involving heterogeneous media, especially fractured media, merit more detailed discussion for three reasons. First, experience shows that fracturing is pervasive in many different geologic settings. Second, the coupling that exists between the fractures and intact rock blocks provides tremendous complexities. Third, substantial information is required to characterize flow and transport processes in fractured media. In general, this information is all but unobtainable with present ground water mensuration technologies.

The earliest combined flow and transport models represented fractured systems either as an equivalent porous medium or as a discrete network of fractures (Schwartz et al., 1983). The first of these approaches assumes that the behavior of the fractured system is describable in a straightforward manner with porous medium models once an appropriate choice of parameters is made. In the second approach, each fracture is represented discretely in terms of its geometry, mean aperture roughness, and interconnection with other fractures. Codes of this type, such as NAPSAC and FracMan/MAFIC (Golder Associates, 1988), have been developed to handle flow and

transport in relatively large and complex fracture networks. They have been applied in assessment of practical fractured rock problems related to the Stripa Project in Sweden.

One limitation of the current generation of discrete fracture codes is the inability to handle fracture-matrix coupling. However, work under way at the University of Waterloo has led to a powerful new modeling approach that incorporates fracture matrix coupling (Sudicky and McLaren, 1992). This work exemplifies the continuing interest in fractured media as applied to many different types of process modeling.

It is beyond the scope of this project to document the numerous initiatives under way to model fractured media. Efforts worthy of special mention, which concern both theoretical and practical aspects of modeling fractured rock systems, are the U.S. Department of Energy sponsored studies at both the Waste Isolation Pilot Plant (WIPP) site in New Mexico and the Yucca Mountain site in Nevada. Given the complexities in both conceptualizing and modeling fractured rock problems, it is not surprising that considerable work remains in this area.

REFERENCES TO CURRENT WORK IN GROUND WATER MODELING

Ground Water Models: Scientific and Regulatory Applications (NRC, 1990) provided a summary of the common solution techniques for problems of fluid flow and solute transport. This summary is expanded in Table 3 to include references to recent modeling advances in special topics: (1) flow and transport in fractured media, (2) optimization, (3) automatic history matching (inverse modeling), (4) multiphase flow, and (5) chemical processes.

TABLE 3 A summary of references to recent advances in modeling for special topics.

	KEY REFERENCES
Flow and Transport in Fractured Media	Endo et al. (1984) Grisale and Pickens (1980) Long and Billaux (1987) Long et al. (1982) Long et al. (1985) Moench (1984) Nitao and Buschek (1991) Preuss and Narasimhan (1985) Schwartz et al. (1983) Shapiro (1987) Shimo and Long (1987) Smith and Schwartz (1984) Smith et al. (1985) Sudicky (1985) Sudicky and Frind (1982) Sudicky and McLaren (1992) Tsang and Tsang (1987) van Genuchten and Dalton (1986) Ward et al. (1989) Witherspoon et al. (1987)
Optimization	Colarullo et al. (1984) Datta and Peralto (1986) GeoTrans (1990) Gorelick (1983) Gorelick and Lefkoff (1985) Gorelick et al. (1984) Greenwald et al. (1992) Lefkoff and Gorelick (1987) Louie et al. (1984) Peralta et al. (1985) Yazdanian and Peralta (1986)

Automatic History Matching (Inverse Modeling)	Carrera (1988) Carrera and Neuman (1984) Carrera and Neuman (1986a) Carrera and Neuman (1986b) Carrera and Neuman (1986c) Cooley (1977) Cooley (1979) Cooley (1982) Cooley and Naff (1990) Faust et al. (1989) Garabedian (1986) Hill (1990) Yeh (1986)
Multiphase Flow	
Vadose Zone	Falta et al. (1989a) Keuper and Frind (1991) Mendoza and Frind (1990) Pruess (1987) Pruess (1991) Sleep and Sykes (1989)
Two-fluid flow	API (1988) EPRI (1988) EPRI (1992) Faust et al. (1989a) Kaluarachchi and Parker (1990) Kuppusamy et al. (1987) McWhorter and Sunada (1990) Parker et al. (1987, 1990) Sleep (1990) Weaver and Charbeneau (1990) Weaver and Charbeneau (in press) Weaver et al. (1992)

Chemical Processes	Davis and Hayes (1986) Degueldre et al. (1989) Hem (1985) Lasaga and Kirkpatrick (1981) Lindberg and Runnells (1984) Liu and Narasimhan (1989) Mangold and Tsang (1991) Mathess and Harvey (1982) Melchior and Bassett (1990) Plummer et al. (1990) Runnells and Lindberg (1990) Ryan and Gschwend (1990) Stumm (1987) Sun and Weeks (1991) Thorstenson (1990) Wierenga (1991)

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Filling the Gaps in the State of Knowledge: Recommendations for Meeting the Army's Modeling Needs

Although considerable progress has already been achieved in several key aspects of ground water modeling, major gaps exist in fundamental knowledge, model development, and site characterization and parameterization. Clearly, the Army cannot address all of the gaps. Instead, the Army should use two criteria to direct its ground water research efforts:

- Emphasize the Army's existing strengths. These strengths include advanced computational capabilities, access to and control over field sites, extensive experience with user interfaces, and a strong background in computational hydraulics.
- Take direct advantage of research and development performed elsewhere, and thus avoid duplicating work already completed or being carried out by others.

These criteria will maximize the impact that the Army's research has on meeting its own needs, as well as contributing to the overall advancement of ground water modeling. Based on this thinking, several recommendations have been identified for an Army program in ground water modeling. These include:

- obtain and develop the necessary expertise for ground water modeling;
- undertake field-scale research and testing of model applications;
- investigate the behavior of explosive chemicals in the subsurface;
- investigate ground water contamination processes in cold climates sites;
- develop state of art user/model interfaces;
- expand the Army/U.S. Amy Corps of Engineers partnership program; and
- develop a ground water modeling support center for research, technology transfer, and training.

These recommendations are not in order of priority, but represent coordinated facets of possible Army research and related activities in ground water modeling. Following the recommendations is a short discussion on the focus of a research program on model parameters.

OBTAIN AND DEVELOP THE NECESSARY EXPERTISE FOR GROUND WATER MODELING

A successful ground water modeling enterprise requires expertise in several disciplines. Modeling involves the use of numerical techniques to solve partial differential equations and thus requires numerical analysts for code development and other functions. But central to the modeling process is someone who understands ground water flow systems, can formulate a conceptual model of the system, and can translate the conceptual model into a numerical model, including boundary and initial conditions. Thus, the critical discipline is usually hydrogeology. A thorough understanding of ground water contaminant processes, problems, and remediation not only involves the science of hydrogeology, but also requires an understanding of microbiology, chemistry, and engineering. Therefore, the application of models to contaminated sites will need a multi-disciplinary team. This suite of expertise is necessary at both the Corps of Engineers district level (major field office), where model applications will be made, and at the research level to improve ground water models. The Army currently does not have staff with the necessary qualifications and will need to hire them.

In addition to obtaining a multidisciplinary staff, the Army should provide adequate opportunity for staff growth and development. In particular, because ground water modeling is a rapidly evolving field being driven by both theoretical developments and the practical need for remediation, it is especially important that staff have ample opportunity to interact with colleagues outside the Army. Journal publication and attendance and participation in conferences should be strongly encouraged. It is very important that an Army initiative in ground water modeling not be isolated from the large and active ground water community.

UNDERTAKE FIELD-SCALE RESEARCH AND TESTING OF MODEL APPLICATIONS

The use of ground water models in the field always involves uncertainty caused by heterogeneity of the subsurface media and by undocumented contaminant sources. In addition, knowledge of which processes are occurring is sometimes uncertain due to limitations of sampling. These types of field-scale uncertainty can be addressed only by field research that explicitly involves modeling. The Army is particularly well positioned to address issues of field-scale uncertainty because it controls many sites located on Army bases. Furthermore, the Army already has considerable capability in site characterization and contaminant analysis. Significant advancements could be made by devoting one or more sites to research for addressing the pressing questions of field-scale uncertainty.

Field-scale research must integrate modeling with site investigation. A field site should be considered a field-scale research laboratory in which processes must be identified and parameter variability evaluated. The levels of site characterization and contaminant monitoring should be established by the needs of model input and uncertainty evaluation. In other words, at a selected set of sites the design of sampling

programs needs to be determined by research goals, not the routine practices of a remedial investigation.

Because models can be used throughout the site characterization and remediation process, which can take years, the Army must develop and implement a strategy to archive modeling studies in a computer data-base format. All too often, modeling studies are performed at a site, but the input data and code are not saved in a way that they can be used for the next phase of the study, and consequently, a new modeling study must be initiated. A strategy to archive the code, input and output files, and calibration information will not only be valuable for the next phase at the site that is modeled, but will also provide technology transfer to model applications at other sites.

INVESTIGATE THE BEHAVIOR OF EXPLOSIVE CHEMICALS IN THE SUBSURFACE

The greatest number of contamination problems at Army sites involve solvents. Other identified contaminants include metals, explosives, hydrocarbons, and pesticides. Although most of the Army's contamination problems are similar to those of the private and public sectors, the problem of contamination by depositories of explosive material has not been studied. It may be that the chemistry involved is sufficiently unique that the Army will need to conduct its own research program to characterize the processes affecting fate and remediation. Scientists at WES are investigating TNT soil sorption dynamics. Research related to explosives should involve site characterization and laboratory studies to identify and quantify physical, chemical, and biological processes occurring in the subsurface. While outside partners will be needed, a substantial effort by Army laboratories appears warranted.

INVESTIGATE GROUND WATER CONTAMINATION PROCESSES IN COLD CLIMATE SITES

Because the Army has bases worldwide, the climate and hydrogeological setting of sites are varied. Investigations into appropriate modeling and remediation approaches for sites in extremely cold climates would also be a useful avenue of research.

DEVELOP STATE-OF-THE-ART USER-MODEL INTERFACES

One of the biggest deterrents to model use in research and practice is the awkwardness of the interface between the user and the model. Specific deficiencies involve access to documentation about the model, input of data, visualization of complex output, and inter-activeness. Those who develop models or sub-models often do not have the skills or resources to implement user-friendly interfaces. On the other hand, the Army, and WES in particular, already has substantial experience with user-model

interfacing, particularly with output visualization. Because the Army's clear need to use ground water models for applied research and field application puts a premium on a friendly user-model interface, a logical direction for the Army is to focus on creating excellent user-model interfaces for the ground water models it uses.

EXPAND THE ARMY/USACE PARTNERSHIP PROGRAM

Fundamental research on the physical, chemical, and biological processes of ground water remediation is carried out at a variety of universities, research institutes, and national laboratories. WES maintains strong academic relations with several universities in environmental engineering and environmental sciences. Army researchers involved with ground water models will need to continue these relations and to establish new long-lasting partnerships with researchers. These partnerships help ensure that advances in fundamental knowledge are incorporated into the models used by the Army and that outside researchers are addressing questions relevant to the Army's needs.

Partnerships can be of several types. Examples include:

- sponsoring research in other laboratories;
- forming research teams, especially for undertaking field-scale research;
- establishing advisory teams in which outside researchers review Army models and applications;
- developing personnel-exchange programs;
- establishing mechanisms by which new research advancements, such as new process sub-models, are incorporated quickly into Army models;
- providing controlled field sites for other researchers to use; and
- serving as a repository and clearinghouse for information and models.

The partnerships will expand the scope of expertise available to the Army, accelerate knowledge transfer to the Army, and provide critical feedback to Army researchers. In addition, they offer an opportunity to close the gap between fundamental research advancements and their incorporation into models.

DEVELOP A SUPPORT CENTER FOR RESEARCH, TECHNOLOGY TRANSFER, AND TRAINING

In regard to site remediation efforts, the position of the U.S. Army is unique in having primary responsibility over an extremely large number of contaminated sites. Furthermore, these sites will require a variety of approaches to ground water modeling. Currently, the Army does not have an adequate force of personnel trained in either research or the application of ground water models to deal with all these sites and situations. While a level of contracting will continue to be necessary, it is unrealistic to expect that adequate supervision of these activities can be done with outside groups.

Therefore, it is important for the Army to develop its capabilities for making full use of ground water modeling techniques, applying the latest research developments, reviewing in-house and contractor model applications, and transferring the technology and expertise within the organization.

Organizationally, there are several ways to approach this problem. One way is to make use of existing partnerships with universities and research centers, and rely on the expertise within academic circles, government, and private industry. One example is the International Ground Water Modeling Center (IGWMC) in Golden, Colorado. While this center does not have a large staff, it is a good source of information on current research and available models, and it provides training courses. The problem with this approach is that it may not be comprehensive enough to reach all Army installations and personnel that require the expertise, and it will be a difficult way to provide leadership and focus for the hundreds of ongoing remediation activities.

A second alternative would be to establish reliance on the U.S. Geological Survey to help with training and technology transfer. While the USGS is an excellent source for information, and may be an appropriate source of support for cooperative studies, it is more likely that USGS would have neither the capacity nor interest in Army-specific problems to be responsive to the Army's mandate for installation remediation.

A third alternative would be for the Army to imitate the USGS model for technology transfer and training. USGS has been successful in using a national center to develop in-house expertise, establish specially designed training courses relevant to its needs, and disseminate information throughout the agency.

Given these alternatives, and the size of the remediation effort at Army installations, the Army should benefit most by developing its own technology transfer and training center for ground water modeling. This would also allow Army-conducted research to be incorporated into the training program. Finally, such a center could serve as a repository to archive site-specific model application data files. The objective here is to create a focal point for both in-house and external research. It is not intended to be the sole source of all work for the Army.

The development of a ground water modeling program requires specialized, multidisciplinary expertise and, ideally, facilities for laboratory work, field experiments, and computer analysis. A centralized approach would support a core of highly qualified personnel who could interact easily and would have access to the resources necessary to implement a coordinated program of laboratory and field scale studies. It should stimulate and facilitate the modeling and cleanup of ground water at Army sites. The proposed center would have research, technology transfer, and training functions. Ideally, the center would have access to sophisticated computing environment, laboratory facilities, training facilities, and to field sites. The Waterways Experiment Station (WES) is a very large complex with some of the most advanced laboratories, field-scale models, and computing facilities in the country dedicated to environmental research and testing. The WES, therefore, seems to be in a position to become equipped to serve as such a center.

A support center would be in a position to serve as a contact point for technology transfer to personnel in the various district offices of the Corps of Engineers engaged in

site-specific ground water modeling tasks and site characterization. Coordination of modeling efforts among the many Army remediation sites could help to further the knowledge base, assist with training activities, and establish standards. Furthermore, the center could help focus the partnership program and act as a conduit for transfer of the latest research developments and application techniques. Recommendations for specific training and technology transfer functions that could be supported through the center include:

- Educate and train district personnel in the proper use of ground water models for Army problems. In this role the Army would have primary responsibility for ensuring that district personnel have adequate training to evaluate ground water problems and to use appropriate ground water models to assist in the solution of those problems. The Army will need new personnel to offer this training function, and it may be appropriate to contract for training staff or to take advantage of the many short-course opportunities currently available.
- Support a core of highly qualified personnel who would advise the districts in site-specific ground water modeling tasks and site characterization. This group would serve as the contact point for the transfer of the latest technology to the districts. The center personnel would serve in advisory and consulting roles for the district offices. These personnel would also provide the additional expertise in ground water modeling that might be needed for tasks that are too large or complex for the personnel or facilities in the district offices.
- Play a central role in identifying the proper technical personnel to deal with site-specific ground water problems of concern to the Army. Such personnel could come from within the center, from the district offices, or from the outside scientific and engineering community. This would help ensure that the "right people are in the right place" to handle Army ground water modeling tasks.
- Serve as an archiving and information-transfer facility. A strategy should be developed to document the use and results of ground water models for Army problems so that the experience gained in one location can be preserved, recovered, and applied to new tasks at other sites. As part of this function, the support center should facilitate internal and external transfer of technology and development of data bases.
- Make every effort to place all data, software, and research results in the unclassified, public domain. Avoid sponsoring external research and development activities that do not lead to publication in the open literature or that lead to non-public domain software.

CONSIDERATIONS OF MODEL PARAMETERS IN DEVELOPING A RESEARCH PROGRAM

It is important to develop a focused research effort on model parameters and on the sources of uncertainty in site characterization. Part of the reason our knowledge of some processes is at the applications stage, as illustrated earlier in Table 1, is because

the controlling parameters are reasonably well understood with a relatively good database of information. Following this logic, it is suggested that major opportunities for research on parameter definition exist in areas of multiphase flow, biological processes, multiphase interactions, coupled flow processes, and fractured media. Through a variety of laboratory and field-scale experiments, the Army has the potential to contribute important new knowledge concerning parameters in contaminated systems. The choice of parameters should be driven by Army cleanup priorities. However, it must be recognized that some processes (e.g., multiphase interactions or coupled flow processes) cannot be easily considered because the number of individual model parameters could be exceedingly large (tens to hundreds of parameters).

Another important aspect of research relating to model parameters is parameter sensitivity. In terms of uncertainty in model predictions, sensitive parameters are of particular importance because small variations in a sensitive parameter can lead to large variations in the model prediction. Thus, in an overall modeling effort, sensitivity analyses with models are extremely helpful in establishing the relative importance of various parameters. This knowledge can serve to establish priorities for the development of new techniques to provide parameter values.

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